

1-Hexene

592-41-6 | DTXSID4025402

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 2.75

Global applicability domain: Inside

Local applicability domain index: 9.97e-01

Confidence level: 8.10e-01

Nearest Neighbors from the Training Set

Image not found

3-Methyl-2-butanone

Measured: 3.04

Predicted: 2.75

Image not found

1-Hexene

Measured: 2.41

Predicted: 2.75

Image not found

Isopropyl ether

Measured: 2.66

Predicted: 2.82

Image not found

Isopropyl acetate

Measured: 2.93

Predicted: 2.76

Image not found

1-Chlorobutane

Measured: 2.72

Predicted: 2.78